Heptane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.56

Global applicability domain: Inside

Local applicability domain index: 6.92e-01

Confidence level: 8.33e-01

Nearest Neighbors from the Training Set

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Heptane
Measured: 4.66
Predicted: 4.56

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Octane
Measured: 5.18
Predicted: 5.05

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n-Hexane
Measured: 3.90
Predicted: 3.96

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(2E)-2-Octene
Measured: 4.51
Predicted: 4.48

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Cycloheptane
Measured: 4.00
Predicted: 4.00